



201-15125

Air Products and Chemicals, Inc.
7201 Hamilton Boulevard
Allentown, PA 18195-1501
Telephone (610) 481-4911

17 December 2003

Via Certified US Mail and e-mail

Administrator
US Environmental Protection Agency
PO Box 1473
Merrifield, VA 22116

Attn: Chemical Right-to-Know Program

RE: Data Analysis, Test Plan and Robust Summaries for 2,4,6-tris[(dimethylamino)methyl]phenol
(CAS # 90-72-2).

Dear Sir:

Air Products and Chemicals, Inc. is pleased to submit the attached data analysis and test plan for 2,4,6-tris[(dimethylamino)methyl]phenol (CAS # 90-72-2) under the U.S. High Production Volume (HPV) Challenge Program. Also attached are robust summaries of the data in an IUCLID-format document.

This submission has also been sent electronically to the following e-mail addresses:

oppt.ncic@epa.gov
chem.rtk@epa.gov

Please contact me at (610) 481-2739 or by e-mail at hamiltce@apci.com if you have questions or if you require additional information.

Regards,

Carrie Hamilton
Toxicology Coordinator
Air Products and Chemicals, Inc.

2 Enclosures

cc w/o attachments: Charles Auer, Director, Chemical Control Division, U.S. EPA
Jim Keith, American Chemistry Council
Charles Bartish, Air Products and Chemicals, Inc.
Bronek Drozdowicz, Air Products and Chemicals, Inc.
Julie O'Brien, Air Products and Chemicals, Inc.

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04 MAR -2 AM 10:25

201-15125A

High Production Volume (HPV) Challenge Program

Data Analysis and Test Plan

For

Phenol, 2,4,6-tris[(dimethylamino)methyl]-

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Prepared by:

Air Products and Chemicals, Inc.
7201 Hamilton Boulevard
Allentown, PA 18195

Submitted: December 2003

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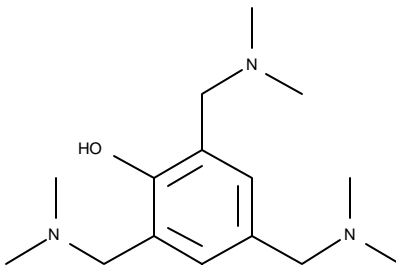
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1.0 INTRODUCTION

Phenol, 2,4,6-tris[(dimethylamino)methyl]- is a Mannich base that is used as a delayed-action gelation catalyst for rigid foams, as a curing agent and as a tertiary amine activator for epoxy resins cured with a wide variety of hardener types. Phenol, 2,4,6-tris[(dimethylamino)methyl]- has the following structure:



Air Products and Chemicals, Inc. has committed to provide basic chemistry, environmental fate, ecotoxicity and health effects information on phenol, 2,4,6-tris[(dimethylamino)methyl]- (CAS 90-72-2) listed under the Environmental Protection Agency (EPA) High Production Volume (HPV) Chemical Challenge Program. By participating in this voluntary program, Air Products and Chemicals, Inc., agreed to assess the adequacy of existing data; prepare summaries of the data characterizing the chemical; determine data needed to fulfill the HPV data requirements; and design and submit a test plan to satisfy these testing requirements.

2.0 EVALUATION OF DATA

2.1 Physico-chemical Data

- 2.1.1 Melting Point:** -20° C (-4° F) [Ref. 1]
- 2.1.2 Boiling Point:** started to decompose at approximately 156° C (313° F) [Ref. 2]
- 2.1.3 Vapor Pressure:** 7.5×10^{-2} Pa @ 25° C (5.6×10^{-4} mm Hg) [Ref. 3]
- 2.1.4 Partition Coefficient:** $\log \text{Pow} = -0.660$ at 21.5° C [Ref. 4]
- 2.1.5 Water Solubility:** >85% w/w (>850 g/l) at 20±0.5° C [Ref. 5]
- 2.1.6 Summary of Physico-chemical Data**

Scientifically reliable data exists for all SIDS physico-chemical endpoints. No additional testing is recommended.

2.2 Environmental Fate and Biodegradation Data

2.2.1 Photodegradation:

Estimation Programs Interface for Microsoft® Windows (EPIWIN V3.10, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, D.C.), Atmospheric Oxidation Program (v1.90) modeling component was used to calculate the rate of photodegradation for phenol, 2,4,6-tris[(dimethylamino)methyl]-. The half-life was calculated to be 0.042 days (or approx. 1/24 hour), assuming the reaction occurred over a 12-hour day with an average atmospheric concentration of 1.5×10^6 OH/cm³ [Ref. 6].

2.2.2 Hydrolysis:

For hydrolysis reactions to occur, there must be an electrophilic carbon atom, which is 'attacked' by oxygen, and a 'leaving group', which departs from the attacked carbon atom. The most electropositive carbon in the phenol, 2,4,6-tris[(dimethylamino)methyl]- molecule is the carbon attached to the phenolic OH group due to the electron withdrawing effect of the phenolic OH group.

The hydrolysis reaction of phenol, 2,4,6-tris[(dimethylamino)methyl]- if it were to occur, would occur by attack of water or OH at the carbon attached to the phenolic OH group. The product of such a reaction would be phenol, 2,4,6-tris[(dimethylamino)methyl]- itself, indicating that there would be no net hydrolysis reaction.

Phenol, 2,4,6-tris[(dimethylamino)methyl]- would be hydrolytically stable under the conditions of the OECD hydrolysis test (OECD Guideline 111), and laboratory testing is not required.

2.2.3 Biodegradation:

Phenol, 2,4,6-tris[(dimethylamino)methyl]- degraded approximately 4% in 28 days in the Closed Bottle test (OECD 301D). Phenol, 2,4,6-tris[(dimethylamino)methyl]- is therefore not readily biodegradable [Ref. 7].

2.2.4 Transport/Distribution:

The Level III fugacity model (from EPIWIN V3.10, US EPA) was used for predicting partitioning of phenol, 2,4,6-tris[(dimethylamino)methyl]- among air, water, soil and sediment compartments. The following are the concentration results using a soil K_{oc} of 0.0897 as calculated by the model and a $\log K_{ow}$ of -0.66 as determined through octanol water partition coefficient testing [Ref. 8]:

- Air <0.01%
- Water 51.9%
- Soil 48%
- Sediment <0.1%

2.2.5 Summary of Environmental Fate and Biodegradation Data

Scientifically reliable data exists for most SIDS environmental fate and biodegradation endpoints. No additional testing is recommended.

2.3 Ecotoxicology Data

2.3.1 Acute Toxicity to Fish:

Phenol, 2,4,6-tris[(dimethylamino)methyl]- was tested in both rainbow trout and carp [Ref. 9].

Rainbow trout (*Salmo gairdneri*) were exposed for 96 hours to concentrations of 0, 140, 180, 240, 280, and 320 mg/l of phenol, 2,4,6-tris[(dimethylamino)methyl]- in a static system. Ten fish were exposed at each concentration. The 24- and 96-hour LC_{50} values (concentration causing 50% of the fish to die) were determined. The 24-hour LC_{50} value was 222 mg/l with a 95 percent confidence interval of 174 to 283 mg/l. The 96-hour LC_{50} value was >180 mg/l but <240 mg/l. The 96-hour LC_{100} value was 240 mg/l. The 96-hour No Observed Effect Level (NOEL) was 180 mg/l.

Carp (*Cyprinus carpio*) were exposed for 96 hours to concentrations of 0, 140, 240, 320, and 420 mg/l of phenol, 2,4,6-tris[(dimethylamino)methyl]- in a static system. Ten fish were exposed at each concentration. The 24- and 96-hour LC_{50} values were determined. The 24-hour LC_{50} value was 249 mg/l with a 95 percent confidence interval of 204 to 305 mg/l. The 96-hour LC_{50} value was 175 mg/l with a 95 percent confidence interval of 131 to 235 mg/l. The 96-hour LC_{100} value was 240 mg/l. The 96-hour NOEL was 140 mg/l.

These results indicate that phenol, 2,4,6-tris[(dimethylamino)methyl]- is practically nontoxic to fish.

2.3.2 Acute Toxicity to Aquatic Invertebrates:

Phenol, 2,4,6-tris[(dimethylamino)methyl]- was tested in both mud crabs and grass shrimp [Ref. 10].

Mud crabs (*Neopanope texana*) were exposed for 96 hours to concentrations of 0, 320, 420, 560, 750, and 1000 mg/l. Ten mud crabs were exposed at each concentration. The 24- and 96-hour LC_{50} values were determined. The 24- and 96-hour LC_{50} values were >750 mg/l but <1000 mg/l. The 96-hour LC_{100} value was 1000 mg/l. The 96-hour NOEL was 750 mg/l.

Grass shrimp (*Palaemonetes vulgaris*) were exposed for 96 hours to concentrations of 0, 320, 420, 560, 750, and 1000 mg/l. Ten shrimp were exposed at each concentration. The 24- and 96-hour LC₅₀ values were determined. The 24-hour LC₅₀ value was >750 mg/l but <1000 mg/l. The 96-hour LC₅₀ was 718 mg/l with a 95 percent confidence interval of 524 to 984 mg/l. The 96-hour NOEL was 560 mg/l.

These results indicate that phenol, 2,4,6-tris[(dimethylamino)methyl]- is practically nontoxic to aquatic invertebrates.

2.3.3 Toxicity to Aquatic Plants:

Phenol, 2,4,6-tris[(dimethylamino)methyl]- has not been tested in algae.

2.3.4 Summary of Ecotoxicology Data

Phenol, 2,4,6-tris[(dimethylamino)methyl]- is practically nontoxic to fish and aquatic invertebrates. Scientifically reliable data exists for these two SIDS ecotoxicity endpoints. Phenol, 2,4,6-tris[(dimethylamino)methyl]- has not been tested in algae. Therefore algal growth inhibition testing according to OECD guideline 201 is recommended.

2.4 Health Effects Data

2.4.1 Acute Health Effects

2.4.1.1 Acute Oral Toxicity

Groups of ten Sprague-Dawley rats (five male and five female) were orally administered undiluted phenol, 2,4,6-tris[(dimethylamino)methyl]- at dose levels of 1333, 2000 and 3000 mg/kg body weight. Surviving animals were observed daily post-dose for 14 days. All animals in the low dose group survived. Three out of ten animals in the mid-dose group died. All animals in the high-dose group died. All surviving animals appeared normal within three days or less of dosing, gained weight, and the only findings seen at necropsy in the survivors were abnormalities of the non-glandular stomach epithelium. Since this material is corrosive, the stomach findings were not unusual. The oral LD₅₀ for phenol, 2,4,6-tris[(dimethylamino)methyl]- in rats was 2169 mg/kg body weight [Ref. 11].

2.4.1.2 Summary of Acute Toxicological Effects

Phenol, 2,4,6-tris[(dimethylamino)methyl]- is practically non-toxic following a single oral exposure. Scientifically reliable data exists for the SIDS acute toxicity endpoint. Additionally this material is corrosive, therefore no additional acute toxicity testing is recommended.

2.4.2 Genetic Toxicology Effects

2.4.2.1 Bacterial Gene Mutation Assay

Phenol, 2,4,6-tris[(dimethylamino)methyl]- diluted in sterile water was examined for mutagenic activity in a *Salmonella typhimurium*-*Escherichia coli* direct plate incorporation assay. The assay was performed using *S. typhimurium* strains TA1535, TA1537, TA98, and TA100 and *E. coli* strain WP2uvrA⁻ over a dose range of 50 to 5,000 ug/plate in both the presence and absence of a phenobarbitone/â-naphthoflavone-induced rat-liver S9 metabolic activation system. OECD guideline 471 was followed. Phenol, 2,4,6-tris[(dimethylamino)methyl]- was not mutagenic under the test conditions used in this bacterial assay. [Ref. 12]

2.4.2.2 In Vitro Chromosomal Aberration Assay

Phenol, 2,4,6-tris[(dimethylamino)methyl]- has not been tested for chromosomal aberrations.

2.4.2.3 Summary of Genetic Toxicology Effects

Phenol, 2,4,6-tris[(dimethylamino)methyl]- was not mutagenic when examined in a *Salmonella typhimurium-Escherichia coli* direct plate incorporation assay according to OECD guideline 471. Phenol, 2,4,6-tris[(dimethylamino)methyl]- has not been tested for chromosomal aberrations. Therefore an in vitro chromosomal aberration test according to OECD guideline 473 is recommended.

2.4.3 Repeated Dose Health Effects

2.4.3.1 Systemic Dermal Toxicity

Rats were exposed dermally to tris(dimethylaminomethyl)phenol at dose levels of 0, 5, 25, and 125 mg/kg/day, 5 days/week for 4 weeks. Treatment-related signs and symptoms included slight to moderate excitability and/or hypertonicity in the 25- and 125-mg/kg, dose groups. Slight to moderate erythema, occasionally accompanied by edema and necrosis, was observed in the 125-mg/kg, dose group. Histopathology revealed moderate to marked hydropic change and slight parakeratosis in the epidermis in the 125-mg/kg, dose group. Slight hydropic change without parakeratosis was noted in the 25-mg/kg, dose group. The no observed effect level (NOEL) was 5 mg/kg/day [Ref. 13].

2.4.3.2 Reproductive and Developmental Toxicity

Phenol, 2,4,6-tris[(dimethylamino)methyl]- has not been tested for reproductive or developmental effects.

2.4.3.3 Summary of Systemic, Reproductive and Developmental Toxicity Effects

Phenol, 2,4,6-tris[(dimethylamino)methyl]- has been evaluated for repeated dose effects via the dermal route of exposure. Due to the corrosive nature of the material, the dose levels employed were relatively low and the clinical and pathological findings were limited to the site of exposure. It is therefore unclear whether phenol, 2,4,6-tris[(dimethylamino)methyl]- would be systemically toxic via oral exposure where a higher dose may be feasible.

Phenol, 2,4,6-tris[(dimethylamino)methyl]- has not been tested for reproductive or developmental effects. Therefore a combined oral repeat dose/repro-screening test according to OECD guideline 422 is recommended.

3.0 CONCLUSIONS

The majority of the data needed to meet the requirements of the HPV program are available and of high quality for phenol, 2,4,6-tris[(dimethylamino)methyl]-. Data for several endpoints are not currently available, therefore additional studies have been recommended to assess the hazards of this chemical. Table 1 shows the studies that exist for phenol, 2,4,6-tris[(dimethylamino)methyl]- and the data that still need to be developed.

TABLE 1: HPV DATA REQUIREMENTS/CRITICAL STUDIES: Phenol, 2,4,6-tris[(dimethylamino)methyl]-

HPV Data Category	Test Endpoint		Acceptable Data Reference (Klimisch Rating)	Data to be Generated
Physical and Chemical Properties	Melting Point		1 (1)	No
	Boiling Point		2 (1)	No
	Vapor Pressure		3 (1)	No
	Partition Coefficient		4 (1)	No
	Water Solubility		5 (1)	No
Environmental Fate and Pathways	Photodegradation		6 (2)	No
	Hydrolysis		NA	No
	Biodegradation		7 (1)	No
	Transport/Distribution		8 (2)	No
Ecotoxicity	Acute toxicity to Fish		9 (2)	No
	Acute toxicity to Aquatic Invertebrates		10 (2)	No
	Toxicity to Aquatic Plants		No	Yes
Human Health Effects	Acute toxicity		11 (1)	No
	Repeated Dose		13 (2)	Yes
	Genetic Toxicity	Gene Mutation	12 (1)	No
		Chromosome Aberration	No	Yes
	Reproductive Toxicity		No	Yes
	Developmental Toxicity		No	Yes

Notes:

Data listed are cross-referenced to a Robust Summary report [i.e. 1 (2)]; which identifies the reference number and Klimisch Rating ().

NA= Not Applicable

4.0 REFERENCES

1. Melting Point: Air Products and Chemicals, Inc. (EXT-03/043). Phenol, 2,4,6-tris[(dimethylamino)methyl]-: Determination of General Physico-Chemical Properties. Testing Facility: Safepharm Laboratories Ltd., Shardlow Derbyshire, UK. Study year: 2003. Klimisch = 1
2. Boiling Point: Air Products and Chemicals, Inc. (EXT-03/043). Phenol, 2,4,6-tris[(dimethylamino)methyl]-: Determination of General Physico-Chemical Properties. Testing Facility: Safepharm Laboratories Ltd., Shardlow Derbyshire, UK. Study year: 2003. Klimisch = 1
3. Vapor Pressure: Air Products and Chemicals, Inc. (EXT-03/057). Phenol, 2,4,6-tris[(dimethylamino)methyl]-: Determination of the Vapor Pressure (OPPTS 830.7950). Safepharm Laboratories Ltd., Shardlow Derbyshire, UK. Study year: 2003. Klimisch = 1
4. Partition Coefficient: Air Products and Chemicals, Inc. (EXT-03/043). Phenol, 2,4,6-tris[(dimethylamino)methyl]-: Determination of General Physico-Chemical Properties. Testing Facility: Safepharm Laboratories Ltd., Shardlow Derbyshire, UK. Study year: 2003. Klimisch = 1
5. Water Solubility: Air Products and Chemicals, Inc. (EXT-03/043). Phenol, 2,4,6-tris[(dimethylamino)methyl]-: Determination of General Physico-Chemical Properties. Testing Facility: Safepharm Laboratories Ltd., Shardlow Derbyshire, UK. Study year: 2003. Klimisch = 1
6. Photodegradation: Estimation Programs Interface for Microsoft® Windows (EPIWIN V3.10, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, D.C.) Atmospheric Oxidation Program (v1.90). Klimisch = 2
7. Biodegradation: Air Products and Chemicals, Inc. (EXT-99/104). Ancamine K54: Assessment of Ready Biodegradability: Closed Bottle Test. Testing Facility: Safepharm Laboratories Ltd., Shardlow Derbyshire, UK. Study year: 1996. Klimisch = 1
8. Transport/Distribution: Estimation Programs Interface for Microsoft® Windows (EPIWIN V3.10, U.S. Environmental Protection Agency, Office of Pollution Prevention and Toxics, Washington, D.C.) Level III Fugacity Model. Klimisch = 2
9. Acute Toxicity to Fish: Air Products and Chemicals, Inc. (EXT-99/034). Acute Toxicity of DMP-30 to Carp (*Cyprinus carpio*), Rainbow Trout (*Salmo gairdneri*), Mud Crab (*Neopanope texana*), and Grass Shrimp (*Palaemonetes vulgaris*). Testing Facility: Bionomics, Inc., Wareham, Massachusetts, USA . Study year: 1973. Klimisch = 2
10. Acute Toxicity to Aquatic Invertebrates: Air Products and Chemicals, Inc. (EXT-99/034). Acute Toxicity of DMP-30 to Carp (*Cyprinus carpio*), Rainbow Trout (*Salmo gairdneri*), Mud Crab (*Neopanope texana*), and Grass Shrimp (*Palaemonetes vulgaris*). Testing Facility: Bionomics, Inc., Wareham, Massachusetts, USA . Study year: 1973. Klimisch = 2
11. Acute Oral Toxicity: Air Products and Chemicals, Inc. (EXT-92/042). Ancamine K54 (BX352): Acute Oral Toxicity Test in the Rat. Testing Facility: Safepharm Laboratories Ltd., Shardlow Derbyshire, UK. Study year: 1992. Klimisch = 1
12. Gene Mutation: Air Products and Chemicals, Inc. (EXT-03/071). Phenol, 2,4,6-Tris[(dimethylamino)methyl]-: Reverse Mutation Assay “Ames Test” Using *Salmonella typhimurium* and *Escherichia coli* (OECD 471). Testing Facility: SafePharm Laboratory, Shardlow, Derbyshire, UK. Study year: 2003. Klimisch = 1
13. Systemic Dermal Toxicity: Initial Submission: Final Report - TK 10433 - 28-Days Dermal Toxicity Study in Rats, EPA/OTS Doc # 88-920007287. Study year: 1986. Klimisch = 2



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7201 Hamilton Boulevard
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Telephone (610) 481-4911

17 December 2003

Via Certified US Mail and e-mail

Administrator
US Environmental Protection Agency
PO Box 1473
Merrifield, VA 22116

Attn: Chemical Right-to-Know Program

RE: Data Analysis, Test Plan and Robust Summaries for 2,4,6-tris[(dimethylamino)methyl]phenol
(CAS # 90-72-2).

Dear Sir:

Air Products and Chemicals, Inc. is pleased to submit the attached data analysis and test plan for 2,4,6-tris[(dimethylamino)methyl]phenol (CAS # 90-72-2) under the U.S. High Production Volume (HPV) Challenge Program. Also attached are robust summaries of the data in an IUCLID-format document.

This submission has also been sent electronically to the following e-mail addresses:

oppt.ncic@epa.gov
chem.rtk@epa.gov

Please contact me at (610) 481-2739 or by e-mail at hamiltce@apci.com if you have questions or if you require additional information.

Regards,

Carrie Hamilton
Toxicology Coordinator
Air Products and Chemicals, Inc.

2 Enclosures

cc w/o attachments: Charles Auer, Director, Chemical Control Division, U.S. EPA
Jim Keith, American Chemistry Council
Charles Bartish, Air Products and Chemicals, Inc.
Bronek Drozdowicz, Air Products and Chemicals, Inc.
Julie O'Brien, Air Products and Chemicals, Inc.

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201-15125B

I U C L I D

Data Set

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Existing Chemical : ID: 90-72-2
CAS No. : 90-72-2
EINECS Name : 2,4,6-tris(dimethylaminomethyl)phenol
EC No. : 202-013-9
Molecular Weight : 265
Structural Formula : C₆H₂[CH₂N(CH₃)₂]₃(OH)
Molecular Formula : C₁₅H₂₇N₃O

Producer related part

Company : Air Products and Chemicals, Inc.
Creation date : 30.01.2003

Substance related part

Company : Air Products and Chemicals, Inc.
Creation date : 30.01.2003

Status :
Memo :

Printing date : 17.12.2003
Revision date :
Date of last update : 17.12.2003

Number of pages : 32

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4
Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1. General Information

Id 90-72-2
Date 17.12.2003

1.0.1 APPLICANT AND COMPANY INFORMATION

Type :
Name : AIR PRODUCTS AND CHEMICALS, INC.
Contact person :
Date :
Street : 7201 HAMILTON BOULEVARD
Town : 18195 Allentown, PA
Country : United States
Phone :
Telefax :
Telex :
Cedex :
Email :
Homepage :

23.10.2003

Type :
Name : Ciba Specialty Chemicals Inc.
Contact person :
Date :
Street :
Town : 4002 Basel
Country : Switzerland
Phone :
Telefax :
Telex :
Cedex :
Email :
Homepage :

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type :
Name : GREAT LAKES CHEMICAL ITALIA
Contact person :
Date :
Street : VIA QUARANTA 29
Town : 20141 MILAN
Country : Italy
Phone : 0039(2)525751
Telefax : 0039(2)52575233
Telex :
Cedex :
Email :
Homepage :

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type :
Name : PROTEX S.A
Contact person :
Date :
Street : 6 rue Barbès
Town : F-92305 LEVALLOIS PERRET
Country : France

1. General Information

Id 90-72-2
Date 17.12.2003

Phone : 33-(1)-47-57-74-00
Telefax : 33-(1)-47-57-69-28
Telex : 46499-0
Cedex :
Email :
Homepage :

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :
Substance type : organic
Physical status : liquid
Purity : ≥ 84 % w/w
Colour :
Odour :

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
15.12.2003

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADE NAMES

2,4,6-Tris[(dimethylamino)methyl]phenol

15.12.2003

Ancamine K54

22.10.2003

Anchor K54

22.10.2003

Araldite Hardener HY960

22.10.2003

Dabco TMR30

1. General Information

Id 90-72-2
Date 17.12.2003

22.10.2003

DMP30

22.10.2003

K54

22.10.2003

1.3 IMPURITIES

Purity :
CAS-No : 71074-89-0
EC-No : 275-162-0
EINECS-Name : bis[(dimethylamino)methyl]phenol
Molecular formula :
Value : < 15 % w/w

15.12.2003

1.4 ADDITIVES

1.5 TOTAL QUANTITY

Quantity : 5000 - 10000 tonnes in
Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

1.6.1 LABELLING

Labelling : as in Directive 67/548/EEC
Specific limits : no data
Symbols : Xn, , ,
Nota : , C,
R-Phrases : (22) Harmful if swallowed
(36/38) Irritating to eyes and skin
S-Phrases : (2) Keep out of reach of children
(26) In case of contact with eyes, rinse immediately with plenty of water
and seek medical advice
(28) After contact with skin, wash immediately with plenty of ...
Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

1.6.2 CLASSIFICATION

Classified : as in Directive 67/548/EEC
Class of danger : corrosive
R-Phrases : (22) Harmful if swallowed
Specific limits :

1. General Information

Id 90-72-2

Date 17.12.2003

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Classified : as in Directive 67/548/EEC
Class of danger : irritating
R-Phrases : (36/38) Irritating to eyes and skin
Specific limits :

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : type
Category : Non dispersive use

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type of use : industrial
Category : Chemical industry: used in synthesis

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type of use : industrial
Category : Polymers industry

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type of use : use
Category : Adhesive, binding agents

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type of use : use
Category : Construction materials additives

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type of use : use
Category : other: catalyseurs pour résines époxydiques, durcisseurs pour polyuréthanes

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

Type of use : use
Category : other: catalyst for epoxide resin systems

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

1. General Information

Id 90-72-2
Date 17.12.2003

11.02.2000

Type of use : use
Category : other

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

Remark : Potential dermal exposure during processing. Use good industrial hygiene practices.
Source : Ciba Specialty Chemicals Inc. Basel
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
12.05.1998

1.11 ADDITIONAL REMARKS

1. General Information

Id 90-72-2
Date 17.12.2003

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2. Physico-Chemical Data

Id 90-72-2
Date 17.12.2003

2.1 MELTING POINT

Value : < -20.2 °C
Sublimation :
Method : other: US EPA OPPTS 830.7200
Year : 2003
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

21.10.2003

(8)

Value : < 0 °C
Decomposition : no, at °C
Sublimation : no
Method : other
Year :
GLP : no data
Test substance :

Source : ANCHOR CHEMICAL(UK)LTD MANCHESTER
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.03.1994

2.2 BOILING POINT

Value : ca. 155.9 °C at 1007.2 hPa
Decomposition : yes
Method : other: US EPA OPPTS 830.7220, ASTM E537-86
Year : 2003
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

15.12.2003

(8)

Value : 130 - 135 °C at 1 hPa
Decomposition : no
Method : other
Year :
GLP : no data
Test substance :

Source : ANCHOR CHEMICAL(UK)LTD MANCHESTER
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

18.03.1994

2.3 DENSITY

Type : relative density
Value : ca. 1.09 g/cm³ at 25 °C
Method : other
Year :
GLP : no data

2. Physico-Chemical Data

Id 90-72-2
Date 17.12.2003

Test substance :
Source : ANCHOR CHEMICAL(UK)LTD MANCHESTER
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
18.03.1994

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .00075 hPa at 25 °C
Decomposition :
Method : other (measured): US EPA OPPTS 830.7950
Year : 2003
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
23.10.2003

(9)

Value : < .01 hPa at 21 °C
Decomposition :
Method : other (measured)
Year :
GLP : no data
Test substance :

Source : ANCHOR CHEMICAL(UK)LTD MANCHESTER
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
18.03.1994

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : = -.66 at 21.5 °C
pH value :
Method : other (measured): US EPA OPPTS 830.7550
Year : 2003
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
23.10.2003

(8)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : ca. 850 g/l at 20 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C

2. Physico-Chemical Data

Id 90-72-2

Date 17.12.2003

Description :
Stable :
Deg. product :
Method : other: US EPA OPPTS 830.7840
Year : 2003
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
13.11.2003

(8)

Solubility in :
Value : ca. 800 g/l at 25 °C
pH value : 11
concentration : 100 g/l at 22 °C

Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : of high solubility

Stable :
Deg. product :
Method : other
Year :
GLP : no
Test substance :

Source : ANCHOR CHEMICAL(UK)LTD MANCHESTER
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
17.12.2003

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : 140 °C
Type : closed cup
Method : Directive 84/449/EEC, A.9 "Flash point"
Year :
GLP : no
Test substance :

Source : ANCHOR CHEMICAL(UK)LTD MANCHESTER
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
18.03.1994

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2. Physico-Chemical Data

Id 90-72-2
Date 17.12.2003

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type : air
Light source :
Light spectrum : nm
Relative intensity : based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : cm³/(molecule*sec)
Degradation : = 50 % after .5 hour(s)
Deg. product :
Method : other (calculated): EPIWIN v3.10, Atmospheric Oxidation Program (v1.90)
Year : 2003
GLP :
Test substance :

Reliability : (2) valid with restrictions
13.11.2003

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type : fugacity model level III
Media :
Air : % (Fugacity Model Level I)
Water : % (Fugacity Model Level I)
Soil : % (Fugacity Model Level I)
Biota : % (Fugacity Model Level II/III)
Soil : % (Fugacity Model Level II/III)
Method : other: EPIWIN v3.10
Year : 2003

Result : Air <0.01%
Water 51.9%
Sediment <0.1%
Soil 48%

Reliability : (2) valid with restrictions
17.12.2003

3.3.2 DISTRIBUTION

3. Environmental Fate and Pathways

Id 90-72-2
Date 17.12.2003

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : aerobic
Inoculum : predominantly domestic sewage
Concentration : 2 mg/l related to Test substance
related to
Contact time : 28 day(s)
Degradation : = 4 (±) % after 28 day(s)
Result : other: not readily biodegradable
Deg. product :
Method : OECD Guide-line 301 D "Ready Biodegradability: Closed Bottle Test"
Year : 1996
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint

17.12.2003

(11)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : static
Species : Cyprinus carpio (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
NOEC : = 140 measured/nominal
LC50 : = 175 measured/nominal
LC100 : = 240 measured/nominal
Method : other: Fish Bioassay Procedure in the 1970 edition of Standard Methods (APHA)
Year : 1973
GLP : no
Test substance :

Method : Fish: Mean weight 0.9 grams; mean length 35 mm

Acclimation period: minimum 30 days

Study was conducted in 5 gallon glass vessels kept in water baths at 21 +/- 1 degree C. Vessels were not aerated.

Standard reconstituted water was prepared by adding 48 mg of NaHCO₃, 30 mg of CaSO₄, 30 mg of MgSO₄, and 2 mg of KCl per liter of deionized water and was used as the standard diluent in the test system.

The pH of the standard diluent was 7.1, and the methyl orange alkalinity was 35 ppm as CaCO₃. Dissolved oxygen values for the various test vessels ranged from 8.8 initially to 4.9 mg/l at the end of the tests.

Result : Signs: Animals generally became dark and lethargic, lost equilibrium, and expired.

Mortality:

Concentration (mg/l)	% Mortality Observed at 24 hours
420	100
320	40
240	50
180	10
140	0
control	0

Concentration (mg/l)	% Mortality Observed at 96 hours
420	100
320	100
240	100
180	80
140	0
control	0

24 hour LC50 = 249 mg/l (95% confidence interval 204-305)

96 hour LC50 = 175 mg/l (95% confidence interval 131-235)

Test substance : DMP-30 (100% active) lot #0978
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
 17.12.2003

(14)

Type : static
Species : Salmo gairdneri (Fish, estuary, fresh water)

4. Ecotoxicity

Id 90-72-2

Date 17.12.2003

Exposure period : 96 hour(s)
Unit : mg/l
NOEC : = 180 measured/nominal
LC50 : 180 - 240 measured/nominal
LC100 : = 240 measured/nominal
Method : other: Fish Bioassay Procedure in the 1970 edition of Standard Methods (APHA)
Year : 1973
GLP : no
Test substance :

Method : Fish: Mean weight 0.8 grams; mean length 40 mm

Acclimation period: minimum 30 days

Study was conducted in 5 gallon glass vessels kept in water baths at 11 +/- 1 degree C. Vessels were not aerated.

Standard reconstituted water was prepared by adding 48 mg of NaHCO₃, 30 mg of CaSO₄, 30 mg of MgSO₄, and 2 mg of KCl per liter of deionized water and was used as the standard diluent in the test system.

The pH of the standard diluent was 7.1, and the methyl orange alkalinity was 35 ppm as CaCO₃. Dissolved oxygen values for the various test vessels ranged from 8.8 initially to 4.9 mg/l at the end of the tests.

Result : Signs: Animals generally became dark and lethargic, lost equilibrium, and expired.

Mortality:

Concentration (mg/l)	% Mortality Observed at 24 hours
320	100
280	100
240	80
180	0
140	0
control	0

Concentration (mg/l)	% Mortality Observed at 96 hours
320	100
280	100
240	100
180	0
140	0
control	0

24 hour LC50 = 222 mg/l (95% confidence interval 174-283)

96 hour LC50 = > 180 < 240 mg/l

Test substance : DMP-30 (100% active) lot #0978
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
17.12.2003

(14)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type : static
Species : Palaemonetes vulgaris (Crustacea)
Exposure period : 96 hour(s)
Unit : mg/l
NOEC : = 560 measured/nominal

4. Ecotoxicity

Id 90-72-2

Date 17.12.2003

EC50 : = 718 measured/nominal
Method : other: Fish Bioassay Procedure in the 1970 edition of Standard Methods (APHA)
Year : 1973
GLP : no
Test substance :

Method : Shrimp: mean length 29 mm

Acclimation period: minimum 10 days

Study was conducted in 2 liters of sea water at 21 +/- 1 degree C. Vessels were not aerated.

Synthetic sea water was used as the standard diluent in the test system.

The pH of the standard diluent was 7.1, and the methyl orange alkalinity was 35 ppm as CaCO₃. Dissolved oxygen values for the various test vessels ranged from 8.8 initially to 4.9 mg/l at the end of the tests.

Remark : A precipitate was present at all concentrations.
Result : Signs: Animals generally became dark and lethargic, lost equilibrium, and expired.

Mortality:

Concentration (mg/l)	% Mortality Observed at 24 hours
1000	60
750	0
560	0
420	0
320	0
control	0

Concentration (mg/l)	% Mortality Observed at 96 hours
1000	100
750	80
560	0
420	0
320	0
control	0

24 hour LC50 = > 750 < 1000 mg/l

96 hour LC50 = 718 mg/l (95% confidence interval 524-984)

Test substance : DMP-30 (100% active) lot #0978
Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
17.12.2003

(14)

Type : static
Species : other aquatic crustacea: mud crab (*Neopanope texana*)
Exposure period : 96 hour(s)
Unit : mg/l
NOEC : = 750 measured/nominal
EC50 : 750 - 1000 measured/nominal
EC100 : = 1000 measured/nominal
Method : other: Fish Bioassay Procedure in the 1970 edition of Standard Methods (APHA)
Year : 1973
GLP : no
Test substance :

Method	: Crab: mean carapace length 15 mm	
	Acclimation period: minimum 10 days	
	Study was conducted in 2 liters of sea water at 21 +/- 1 degree C. Vessels were not aerated.	
	Synthetic sea water was used as the standard diluent in the test system.	
	The pH of the standard diluent was 7.1, and the methyl orange alkalinity was 35 ppm as CaCO ₃ . Dissolved oxygen values for the various test vessels ranged from 8.8 initially to 4.9 mg/l at the end of the tests.	
Remark	: A precipitate was present at all concentrations.	
Result	: Signs: Animals generally became dark and lethargic, lost equilibrium, and expired.	
	Mortality:	
	Concentration (mg/l)	% Mortality Observed at 24 hours
	1000	100
	750	0
	560	0
	420	0
	320	0
	control	0
	Concentration (mg/l)	% Mortality Observed at 96 hours
	1000	100
	750	0
	560	0
	420	0
	320	0
	control	0
	24 hour LC50 = > 750 < 1000 mg/l	
	96 hour LC50 = > 750 < 1000 mg/l	
Test substance	: DMP-30 (100% active) lot #0978	
Reliability	: (2) valid with restrictions	
Flag	: Critical study for SIDS endpoint	
17.12.2003		

(14)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE**4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA****4.5.1 CHRONIC TOXICITY TO FISH****4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES****4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS**

4. Ecotoxicity

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4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 2169 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	10
Vehicle	:	
Doses	:	
Method	:	OECD Guide-line 401 "Acute Oral Toxicity"
Year	:	1987
GLP	:	yes
Test substance	:	other TS
Method	:	TEST ORGANISMS: <ul style="list-style-type: none">- Source: Charles River (UK) Ltd.- Age: 5-8 weeks- Number: 5/sex/dose- Weight at study initiation: males 126-148 g, females 120-142 g ADMINISTRATION: <ul style="list-style-type: none">- Doses: 1333, 2000, and 3000 mg/kg bw- Doses per time period: single dose by gavage- Volume administered or concentration: 1.38-3.10 ml/kg bw- Post dose observation period: 14 days EXAMINATIONS: <ul style="list-style-type: none">- clinical signs and mortality: 0.5, 1, 2 and 4 hours after dosing and subsequently once daily for 14 days- body weight: day 0, 7 and 14 (or at death)- macroscopy STATISTICAL METHOD: <ul style="list-style-type: none">- Thompson, 1947
Result	:	MORTALITY: <ul style="list-style-type: none">- Number of deaths at each dose (time of death): at 1333, 2000 and 3000 mg/kg: 0, 1 male (day 4)/2 females (day 1), 10 (day 1) CLINICAL SIGNS: <ul style="list-style-type: none">- At 1333 mg/kg hunched posture; at 2000 mg/kg lethargy and/or hunched posture and decreased respiratory rate and labored breathing in the male that died. All animals were recovered by day 3; at 3000 mg/kg lethargy, comatosis, ptosis, ataxia, and hunched posture, decreased respiratory rate and red/brown stains around the snout in one male- body weight decreased in animals that died and at 2000 mg/kg NECROPSY FINDINGS: <ul style="list-style-type: none">- At 1333 mg/kg large amounts of white foci scattered over nog-glandular epithelium of stomach; at 2000 mg/kg (in animals that died) and 3000 mg/kg hemorrhagic and red

5. Toxicity

Id 90-72-2

Date 17.12.2003

	stained lungs, dark or patchy pallored liver, dark colored kidneys, hemorrhagic gastrous mucosa and non-glandular stomach epithelium, gaseous distension or severe hemorrhage of small and large intestine; surviving animals at 2000 mg/kg displayed foci on stomach epithelium.	
Test substance	: Other, CAS 90-72-2 (phenol, 2,4,6-tris[(dimethylamino)methyl], purity 97%	
Conclusion	: LD50: Combined sexes 2169 (1916-2455) mg/kg bw Males: 2259 (1920-2656) mg/kg bw Females: 2083 (1707-2540) mg/kg bw	
Reliability Flag	: (1) valid without restriction : Critical study for SIDS endpoint	
13.11.2003		(6)
Type	: LD50	
Value	: = 1673 mg/kg bw	
Species	: rat	
Strain	: other: CFY strain	
Sex	: male/female	
Number of animals	: 10	
Vehicle	: other: undiluted	
Doses	:	
Method	: other: not specified	
Year	: 1975	
GLP	: no	
Test substance	: other TS	
Method	: TEST ORGANISMS: - Number: 5 males + females - Weight at study initiation: males 200-203 g, females 201-209 - Controls: 5 males + 5 females treated with water (4 ml/kg) ADMINISTRATION: - Doses: 0.64, 1, 1.6, 2.5, 4 g/kg (based on rel density of 0.97; 0.64-4 ml/kg) - Doses per time period: 1 - Postdose observation period: 14 days EXAMINATIONS: - mortality and signs of toxicity - body weight: at start of the study, and after 7 and 14 days - all rats were examined macroscopically STATISTICAL METHOD: - Weil C.S. (1952)	
Result	: MORTALITY: - Number of deaths at each dose (hours after dosing): at 0, 0.64, 1 g/kg: 0/10; at 1.6 g/kg: 4/5 females (<26); at 2.5 g/kg 10/10 (< 5 males, < 3 females) and 4 g/kg: 10/10 (<5). CLINICAL SIGNS: - Pilerection and slightly increased salivation (at 1 and 4 ml/kg); lethargy and body tremors (at 1.6, 2.5, and 4 ml/kg); ataxia (3/5 females at 1.6 ml/kg). Recovery of survivals was apparently complete within 7 days after treatment. BODY WEIGHT gain was depressed after 7 days, but normal after 14 days.	

		<p>NECROPSY FINDINGS:</p> <ul style="list-style-type: none"> - Rats that died: severe hemorrhage of the stomach and intestine, injection of the mesenteric blood vessels, market distension of the large intestine, darkening of the liver (generally accompanied by slight lung hemorrhage). - Survivals: no abnormalities. 	
Test substance	:	Other, CAS 90-72-2 (phenol, 2,4,6-tris[(dimethylamino)methyl] purity: 97%, with 0.5% water.	
Conclusion	:	LD50: 1673 mg/kg bw; 95% confidence limits: 1378-1968 mg/kg bw.	
Reliability 15.12.2003	:	(2) valid with restrictions	(4)
Type	:	LD50	
Value	:	2400 - 2600 mg/kg bw	
Species	:	rat	
Strain	:		
Sex	:		
Number of animals	:		
Vehicle	:		
Doses	:		
Method	:	OECD Guide-line 401 "Acute Oral Toxicity"	
Year	:		
GLP	:	no data	
Test substance	:	other TS	
Source	:	ANCHOR CHEMICAL(UK)LTD MANCHESTER EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)	
Reliability 17.12.2003	:	(4) not assignable	(16)
Type	:	LD50	
Value	:	1000 - 1340 mg/kg bw	
Species	:	rat	
Strain	:		
Sex	:		
Number of animals	:		
Vehicle	:		
Doses	:		
Method	:	OECD Guide-line 401 "Acute Oral Toxicity"	
Year	:		
GLP	:	no data	
Test substance	:	other TS	
Source	:	ANCHOR CHEMICAL(UK)LTD MANCHESTER EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)	
Reliability 17.12.2003	:	(4) not assignable	(16)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	ca. 1280 mg/kg bw
Species	:	rat

5. Toxicity

Id 90-72-2

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Strain :
Sex :
Number of animals :
Vehicle :
Doses :
Method : OECD Guide-line 402 "Acute dermal Toxicity"
Year :
GLP : no data
Test substance : other TS

Source : ANCHOR CHEMICAL(UK)LTD MANCHESTER
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (4) not assignable
15.12.2003

(17)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
Vehicle :
PDII :
Result : corrosive
Classification : corrosive (causes burns)
Method : OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year : 1992
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Source : ANCHOR CHEMICAL(UK)LTD MANCHESTER
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (1) valid without restriction
17.12.2003

(1)

Species : rabbit
Concentration :
Exposure :
Exposure time :
Number of animals :
Vehicle :
PDII :
Result : corrosive
Classification : corrosive (causes burns)
Method : other: DOT TEST
Year : 1983
GLP : yes
Test substance : other TS: Dabco TMR 30

Source : ANCHOR CHEMICAL(UK)LTD MANCHESTER
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Reliability : (1) valid without restriction
17.12.2003

(7)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration :
Dose :
Exposure time :
Comment :
Number of animals :
Vehicle :
Result : highly irritating
Classification : irritating
Method : other: CFR TITLE 16,SEC.1500.42
Year : 1975
GLP : no data
Test substance : as prescribed by 1.1 - 1.4

Source : ANCHOR CHEMICAL(UK)LTD MANCHESTER
 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Reliability : (2) valid with restrictions
 17.12.2003

(2)

5.3 SENSITIZATION

Type : Guinea pig maximization test
Species : guinea pig
Concentration : 1st: Induction .05 % intracutaneous
 2nd: Induction 25 % occlusive epicutaneous
 3rd: Challenge 2 % occlusive epicutaneous

Number of animals : 30
Vehicle : water
Result :
Classification : not sensitizing
Method : OECD Guide-line 406 "Skin Sensitization"
Year : 1995
GLP : yes
Test substance : as prescribed by 1.1 - 1.4

Method : Based on the results of sighting tests, the following concentrations of Ancamine K54 in distilled water were used: 0.05% w/v for the intradermal induction, 25% v/v for the topical induction, and 2% and 1% v/v for the topical challenge.

 Animals:
 Forty male, albino Dunkin Hartley guinea pigs supplied by David Hall Limited, Burton-on-Trent, Staffordshire, UK were used. At the start of the main study the animals weighed 306 to 401g, and were approximately eight to twelve weeks old.

 Twenty test and ten control animals were used for the main study.

Result : Two animals exhibited very slight erythema at the 2% v/v challenge site at the 24-hour observation. No skin reactions were noted at the 48-hour observation. Ancamine K54 produced an 11% (2/19) sensitization rate and is a mild sensitizer to guinea pig skin.

Reliability : (1) valid without restriction
Flag : Critical study for SIDS endpoint
 15.12.2003

(5)

Type : Buehler Test
Species : guinea pig

Number of animals	: 78
Vehicle	:
Result	: not sensitizing
Classification	: not sensitizing
Method	: OECD Guide-line 406 "Skin Sensitization"
Year	:
GLP	: no data
Test substance	: other TS
Method	: Animals: Seventy eight (39 male / 39 female) young adult Hartley guinea pigs
	Eight guinea pigs (4 male, 4 female) were assigned to a preinduction primary skin irritation study.
	The induction phase consisted of ten 6-hour applications (3 doses/week) over 3 weeks. Four groups of 10 guinea pigs received 0.4 ml of DMP-30 at w/v concentrations of 0.3, 1.0, 3.0 or 10% in distilled water. A group of 10 guinea pigs was treated with 0.4 ml of 1-chloro-2,4-dinitrobenzene (DNCB) at 0.1% w/v (1000 ppm) concentration in 80% aqueous ethanol in the same manner and served as the positive control group. An additional group of 10 animals were sham treated. The six groups were challenged 14 days after the last induction dose/treatment. The DMP-30 groups were challenged with 0.4 ml of DMP-30 at 1.0, 3.0, and 10% w/v in distilled water. The positive control group received a challenge dose of 1000 ppm DNCB in acetone (0.4 ml). The sham treatment (noninduced) control group was challenged with 1.0, 3.0, and 10% DMP-30 in distilled water and 1000 ppm DNCB in acetone (0.4 ml each). Twelve days after the primary challenge, the induced groups of guinea pigs were rechallenged with DMP-30 at concentrations of 1.0 and 10% in distilled water, and the positive control group was rechallenged with DNCB at 1000 ppm in acetone. Similarly an additional naive control group of ten guinea pigs was challenged with DNCB at 1000 ppm in acetone and DMP-30 at 1.0 and 10% w/v distilled water.
Result	: The sporadic incidence of dermal reactions in the DMP-30 test groups after challenge and rechallenge and in one naive control animal after rechallenge are attributed to a local primary irritation response. Erythema responses were not consistently dose related and not found in the same DMP-30 treated animals in both phases.
Source	: ANCHOR CHEMICAL(UK)LTD MANCHESTER EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance	: DMP-30, Lot #6-5708
Reliability	: (1) valid without restriction
13.11.2003	(15)

5.4 REPEATED DOSE TOXICITY

Type	:
Species	: rat
Sex	: male
Strain	: Sprague-Dawley
Route of admin.	: dermal
Exposure period	: 14 days
Frequency of treatm.	: once per day
Post exposure period	: 1 day post-mortum examination
Doses	: 1.0 and 0.1 ml/kg/day; 8 animals per group.
Control group	: yes, concurrent no treatment
Method	: other
Year	: 1983
GLP	: yes

Test substance	: as prescribed by 1.1 - 1.4	
Result	: No deaths occurred during the study. However at a dose of 1.0 ml/kg/day the test article produced a very severe skin response consisting of extensive eschar formation and ulceration. This exposure was so severe that treatment was discontinued after 4 days, both to avoid unnecessary suffering and because there was insufficient unaltered skin to which treatment could be applied. Treatment with the test article at 0.1 ml/kg/day produced a mild irritant response characterised by a slight erythema 24 hours after treatment and occasional slight eschar formation. As the animals were obtained as adults there was little body-weight gain during the study. However, the body weights of the group given 0.1 ml test article per day were statistically significantly lower than those of controls on most occasions during the study, and the animals treated at 1.0 ml/kg/day for four days showed a weight loss during this period that was only partially regained subsequently. Observation of the animals throughout the study did not reveal any other treatment-related differences either in appearance or behaviour. At post-mortem examination no difference was seen between treated and control animals in the appearance of any of the tissues apart from the treated areas of skin.	
Source	: ANCHOR CHEMICAL(UK)LTD MANCHESTER EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)	
17.12.2003		(3)
Type	:	
Species	: rat	
Sex	:	
Strain	:	
Route of admin.	: dermal	
Exposure period	: 4 weeks	
Frequency of treatm.	: 5 times a week	
Post exposure period	:	
Doses	: 0, 5, 25, or 125 mg/kg	
Control group	:	
NOAEL	: = - 5 mg/kg	
Method	:	
Year	: 1986	
GLP	:	
Test substance	: other TS	
Result	: The test substance was applied to the skin of rats 5 times a week for 4 weeks at daily doses of 0, 5, 25, or 125 mg/kg. Treatment-related signs and symptoms included slight to moderate excitability and/or hypertonicity in the 25 and 125 mg/kg dose groups. Slight to moderate erythema, occasionally accompanied by slight, transient edema and necrosis, was recorded in the 125 mg/kg group. The irritation disappeared before the end of treatment. Histopathology revealed moderate to marked hydropic change and slight parakeratosis in the epidermis in the 125 mg/kg dose group. Slight hydropic changes without obvious parakeratosis was recorded in the 25 mg/kg group.	
Test substance	: The no-observed effect level (NOEL) was 5 mg/kg. Tris(dimethylaminomethyl)phenol (Hardener HY960)	
17.12.2003		(12)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	: Ames test
System of testing	: TA98, TA100, TA1535, TA1537, and Escherichia coli strain WP2uvrA
Test concentration	: 50 to 5000 ug/plate
Cycotoxic concentr.	: None
Metabolic activation	: with and without
Result	: negative
Method	: OECD Guide-line 471
Year	: 2003
GLP	: yes
Test substance	: as prescribed by 1.1 - 1.4
Method	: Vehicle: sterile distilled water
Result	Metabolizing system: 10% liver S9 in standard co-factors : No test material precipitate was observed at any dose. No visible reduction in the growth of the bacterial background lawn was observed at any dose. No significant increases in the frequency of revertant colonies were recorded for any of the bacterial strains at any dose.
Reliability	: (1) valid without restriction
Flag	: Critical study for SIDS endpoint
17.12.2003	(10)
Type	: Ames test
System of testing	: TA98 and TA100
Test concentration	: 100 ul
Cycotoxic concentr.	:
Metabolic activation	: with and without
Result	: negative
Method	: other: not indicated
Year	:
GLP	: no data
Test substance	: other TS
Test substance	: Other, DMP-30, CAS 90-72-2 (Phenol, 2,4,6-tris[(dimethylamino)methyl]), purity not indicated
Reliability	: (4) not assignable Overview article about epoxy resins used in the electron microscopy, with minor information.
17.12.2003	(13)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5. Toxicity

Id 90-72-2
Date 17.12.2003

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7. Eff. Against Target Org. and Intended Uses

Id 90-72-2
Date 17.12.2003

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

- (1) APCI (Anchor Chemical Limited), Ancamine K54 (BX352): Acute Dermal Irritation Test in the Rabbit, unpublished study, APCI RRRS EXT -92/043
- (2) APCI (Anchor Chemical Limited), Ancamine K54 Irritant Effects on Rabbit Eye Mucosa, unpublished study, APCI RRRS EXT -91/111
- (3) APCI (Anchor Chemical Limited), Ancamine K54: Report of a 14-Day Percutaneous Toxicity Study in the Rat, APCI RRRS EXT-03/076
- (4) APCI (Anchor Chemical Limited), Ancamine K54: Acute oral toxicity to rats, 1975, unpublished study, APCI RRRS EXT -91/112
- (5) APCI (Anchor Chemical Limited), Ancamine K54: Magnusson & Kligman Maximization Study in the Guinea Pig, unpublished study, APCI RRRS EXT-96/015
- (6) APCI (Anchor Chemical Limited), Curing Agent K54 (BX352): Acute oral toxicity test in the rat, unpublished study, APCI RRRS EXT -92/042
- (7) APCI, Dabco TMR-30: DOT Corrosivity Test, unpublished study, APCI RRRS EXT-83/006
- (8) APCI, Phenol, 2,4,6-tris[(dimethylamino)methyl]: Determination of General Physico-Chemical Properties, unpublished study, APCI RRRS EXT -03/043
- (9) APCI, Phenol, 2,4,6-tris[(dimethylamino)methyl]: Determination of Vapor Pressure (OPPTS 830.7950), unpublished study, APCI RRRS EXT -03/057
- (10) APCI, Phenol, 2,4,6-tris[(dimethylamino)methyl]: Reverse Mutation Assay "Ames Test" Using Salmonella Typhimurium and Escherichia Coli (OECD 471), unpublished study, APCI RRRS EXT-03/071
- (11) APME Epoxy Resin Committee, Ancamine K54: Assessment of Ready Biodegradability - Closed Bottle Test (OECD 301D), unpublished study, APCI RRRS EXT-99/104
- (12) Ciba-Geigy 8EHQ-0892-8893
- (13) Murray P., Mutagenic activity of epoxy embedding reagents employed in electron microscopy, 1979
- (14) Rohm & Haas Company, Acute Toxicity of DMP-30 To Carp (Cyprinus carpio) Rainbow Trout (Salmo gairdneri), Mud Crab (Neopanope txana), and Grass Shrimp (Palaemonetes vulgaris), unpublished study, APCI RRRS EXT -99/034
- (15) Rohm & Haas Company, DMP -30: Delayed Contact Hypersensitivity Study in Guinea Pigs, Report 88RC-0084 dated 2/7/89.
- (16) Rohm & Haas Company, Summary of Toxicological Data on DMP -30, unpublished studies, APCI RRRS EXT-93/011
- (17) V. A. Volodchenko and E.R. Sadokha, Comparative toxicology of 2,4,6-tris(dimethylaminomethyl)phenol trioleate and 2,4,6-tris(dimethylaminomethyl)phenol, new curing agents for epoxy resins., Farmakol. i Toksikol. Vol. 37 [3], 363-4 (1974)

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT